

## **A Framework for a Computational Toxicology Research Program in ORD**

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**Key Words:** computational toxicology, risk assessment, molecular biology, computational chemistry, hazardous chemicals

Computational Toxicology (CompTox) is a new emerging research program in ORD targeted at improving hazard and risk assessment. Operationally, CompTox is defined as the integration of modern computing and information technology with modern molecular chemistry and biology, with the goal of improving Agency prioritization of data requirements and risk assessments of chemicals. In the broadest sense, it will attempt to provide tools and approaches that will help define which chemicals need testing for which outcomes and in what sequence. Thus, it has applicability to a number of regulatory activities such as those involving hazardous air pollutants, candidate contaminant lists, endocrine disruptors, pesticidal inerts, and non-food use anti-microbial agents. The effort is guided by a steering group (the CTISC) composed of members of all of the labs and centers and is titled "A Framework for a Computational Toxicology Research Program in ORD," which has received SAB and BOSC review and consultation. The CompTox program has identified three long-term objectives for its activity: improving the linkages in the source-to-outcome paradigm so as to increase the predictive nature of our measures, providing predictive models for screening and testing, and enhancing quantitative risk assessment. A number of technology-based tools, such as genomics, proteomics, metabonomics, and systems biology, are being explored as means to achieve the objectives. Due to the magnitude of the task, it is essential that the program works closely with the intramural investigators, the STAR program, and external partners to bring sufficient breadth of expertise and resources to bear on the identified issues. Initial efforts are being focused on a number of "proof-of-concept" studies to demonstrate the effectiveness of the approach. These studies include endocrine disruptor screening methodologies, predictive toxicogenomic models of hepatotoxicity, and comparative in vitro/in vivo expression analyses. Activities related to the CompTox program are available on the Internet ([www.epa.gov/comptox](http://www.epa.gov/comptox)), and a quarterly communiqué is being planned for broad distribution. This poster discussion session was designed to highlight progress being made in implementing various aspects of the Framework.